# Density of states: 2D

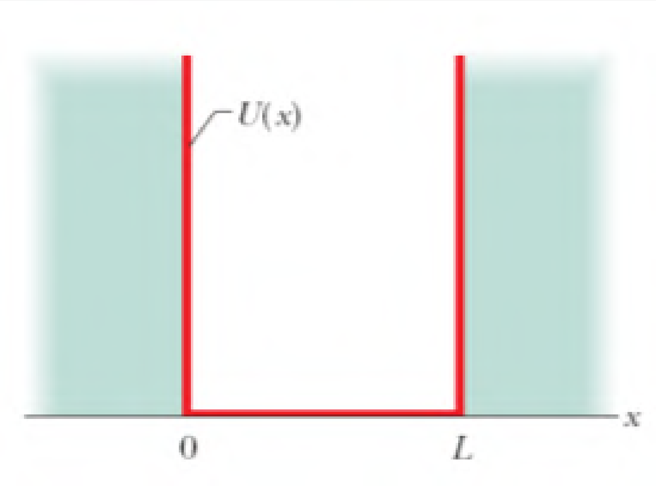
**Outlines:**

1. Introduction of 2D, 1D and 0D materials
2. Density of state of 2D (Quantum Well)
3. Problems based on density of state

# Prerequisite/Recapitulations

Electron trapped in 1D infinite potential box and quantization of energy:

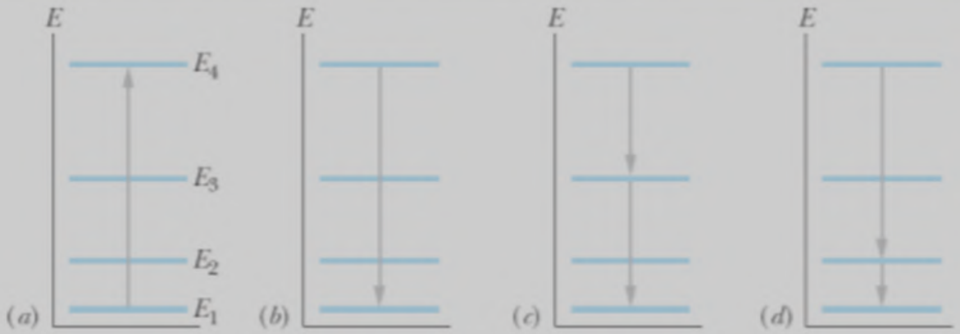
$$E_n = \left(\frac{h^2}{8mL^2}\right)n^2, \qquad \text{for } n = 1, 2, 3, \ldots .$$




$$\Delta E = E_{high} - E_{low}.$$

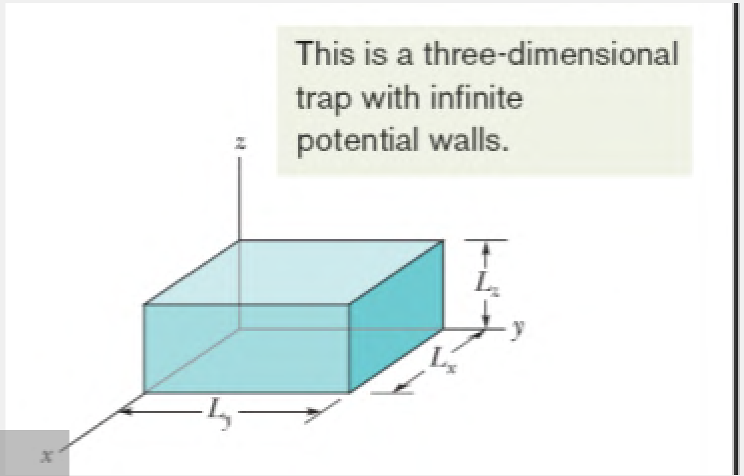
The electron is excited to a higher energy level.

It can de-excite to a lower level in several ways (set by chance).



# Prerequisite/Recapitulations

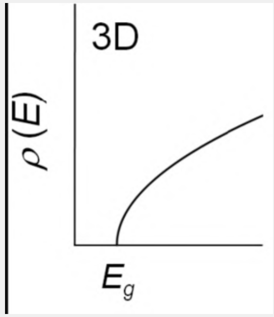
A basic characteristic of all matter at the low dimension/nano scale is the manifestation of the wave–particle duality—a fundamental quantum-mechanical principle that states that all matter (electrons, nuclei, photons, etc.) behaves as both waves and particles.. The quantum effects of confinement become significant when at least one of the dimensions of a structure is comparable in length to the de Broglie wavelength. If at least one dimension of a solid is comparable to the de Broglie wavelength of the particle, a quantum-mechanical treatment of particle motion becomes necessary.




Energy of electron trapped in 3D infinite potential box:

The energy of an electron trapped in a 3-D infinite potential box:

$$E_{nx,ny,nz} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right).$$




Basics of density of state:The density of states function describes the number of states that are available in a system and is essential for determining the carrier concentrations and energy distributions of carriers within a semiconductor.

# Learning outcome:

After the completion of this lecture you will be able to:

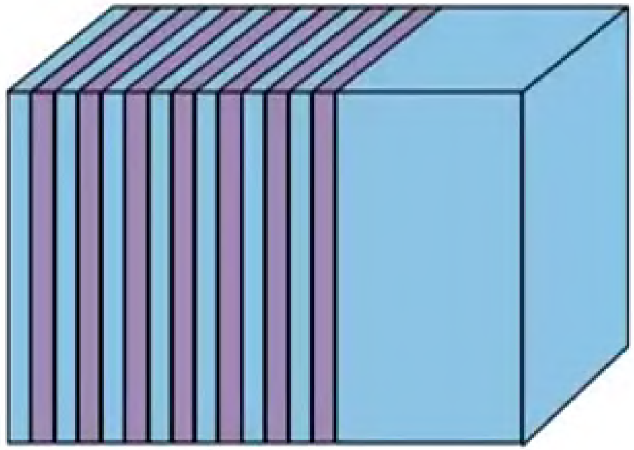
1. Explain the density of states in solids

2. Interpret the quantum well, quantum wire and quantum dots

3. Derive the density of state of quantum well

# Conceptualization

## Quantum well structures



# Introduction

Quantum wires and quantum dots are two and three dimensional analogs of the conventional quantum well

A quantum dot, for example, would confine an electron in three dimensions to a size comparable to the de Broglie wavelength of the electron in the crystal.

The most important property of quantum wires and quantum dots as concerns their application to laser diode.

# Introduction

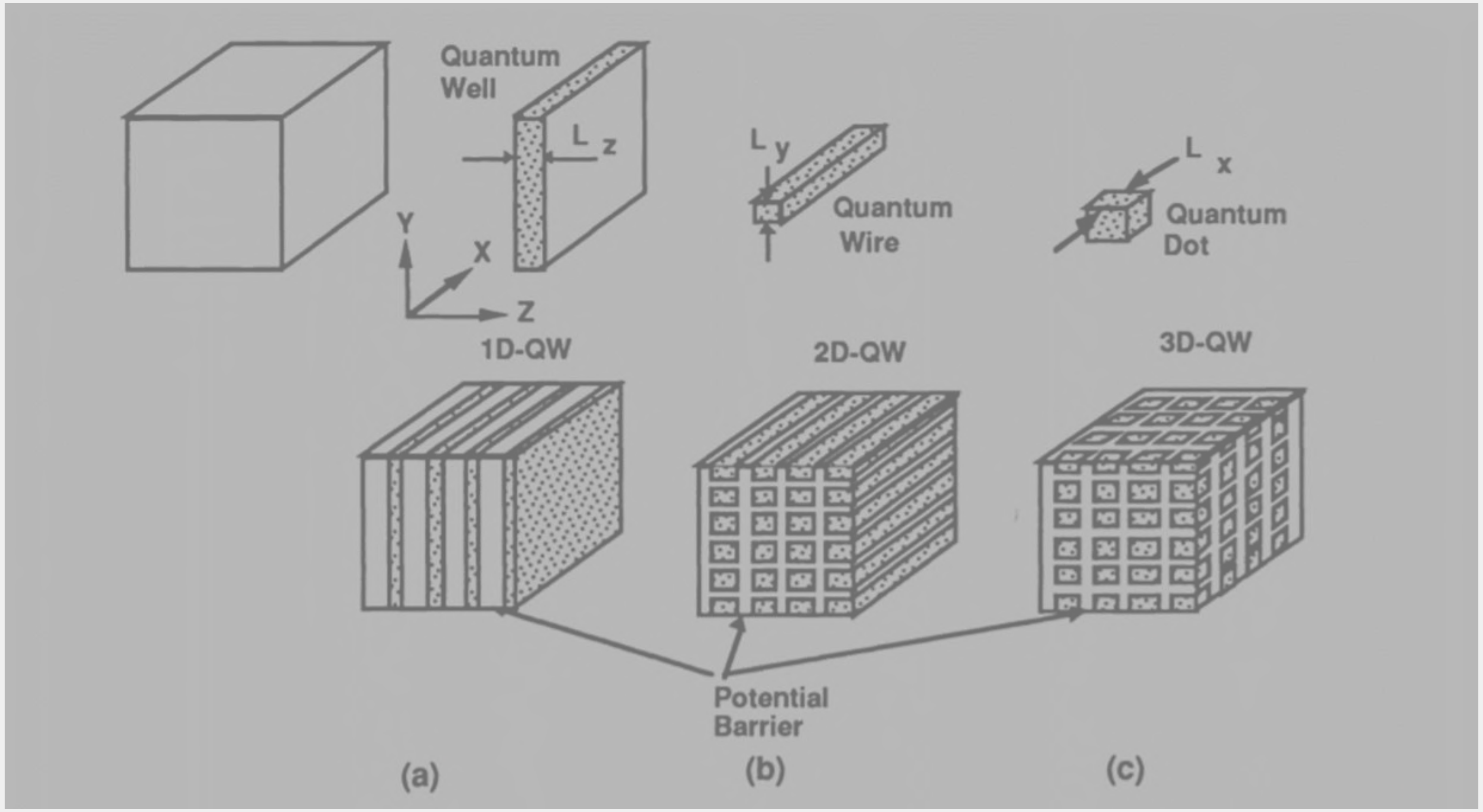
**Three-dimensional (3D) structure or bulk structure:** No quantization of the particle motion occurs, i.e., the particle is free.

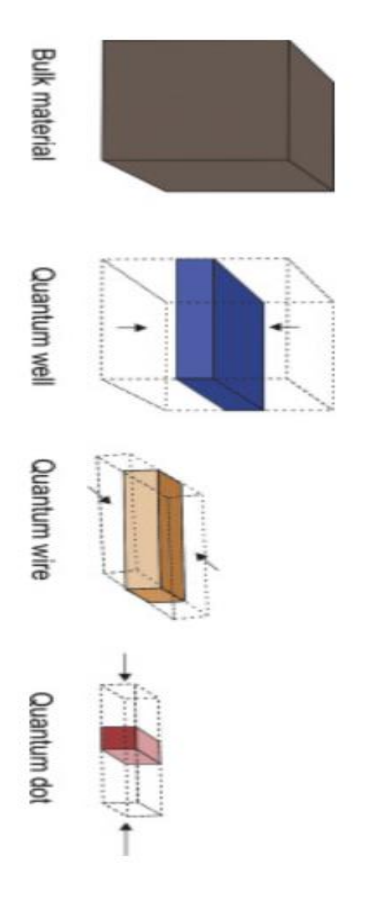
**Two-dimensional (2D) structure or quantum well**: Quantization of the particle motion occurs in one direction, while the particle is free to move in the other two directions.

**One-dimensional (1D) structure or quantum wire**: Quantization occurs in two directions, leading to free movement along only one direction.

**Zero-dimensional (0D) structure or quantum dot (sometimes called "quantum box")**: Quantization occurs in all three directions

# Quantum wells, wires and dots

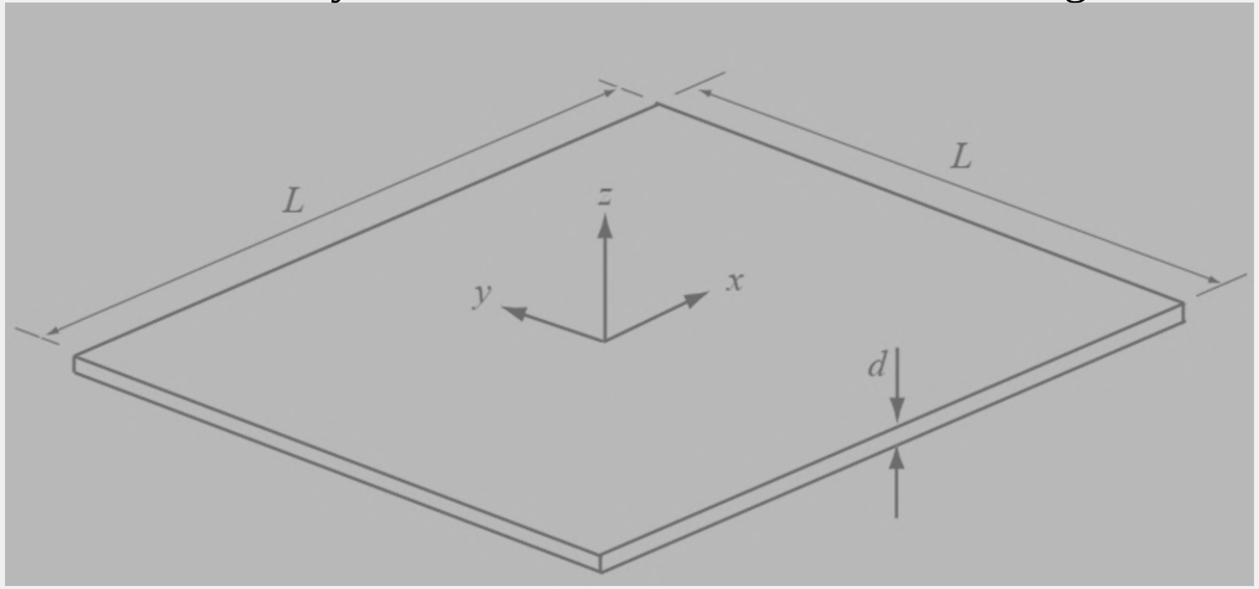



Quantum wells, wires and dots showing the successive dimensions of confinement .

# Quantum Well (2D)

Quantum effects arise in systems which confine electrons to regions comparable to their de Broglie wavelength. When such confinement occurs in one dimension only (say, by a restriction on the motion of the electron in the *z*-direction), with free motion in the *x*- and *y*-directions, a two-dimensional system is created, which is shown in Figure



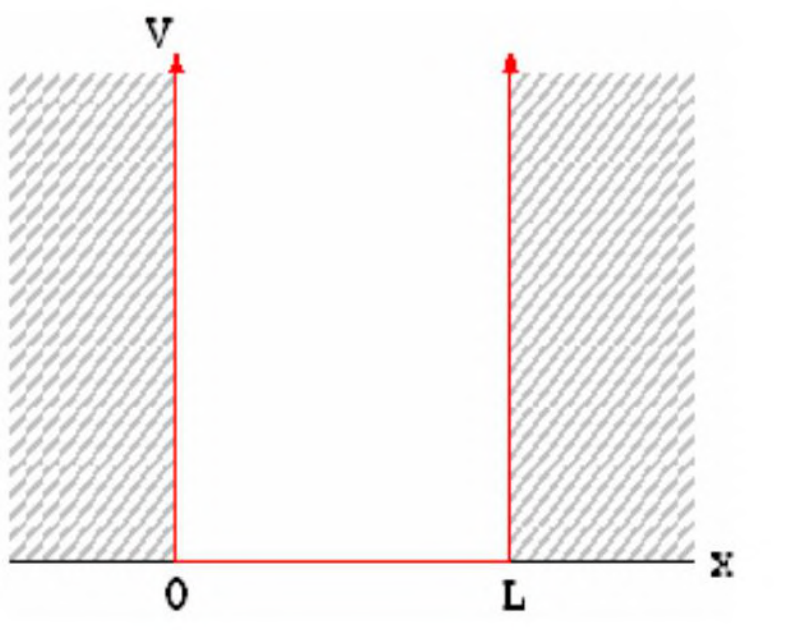
# Derivation of density of state of Quantum well (2D)

We can model a semiconductor as an infinite quantum well (2D) with sides of length L. Electrons of mass m are confined in the well.
If we set the PE in the well to zero, solving the Schrödinger equation yields

$$\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+k^2\psi = 0$$

$$where\ k = \sqrt{\frac{2mE}{\hbar^2}}$$



# Derivation of density of state of Quantum well (2D)

The solutions to the wave equation where V(x) = 0 are sine and cosine functions

$$\psi = A\sin(k_x x) + B\cos(k_x x)$$

Since the wave function equals zero at the infinite barriers of the well, only the sine function is valid. Thus, only the following values are possible for the wave number (k)

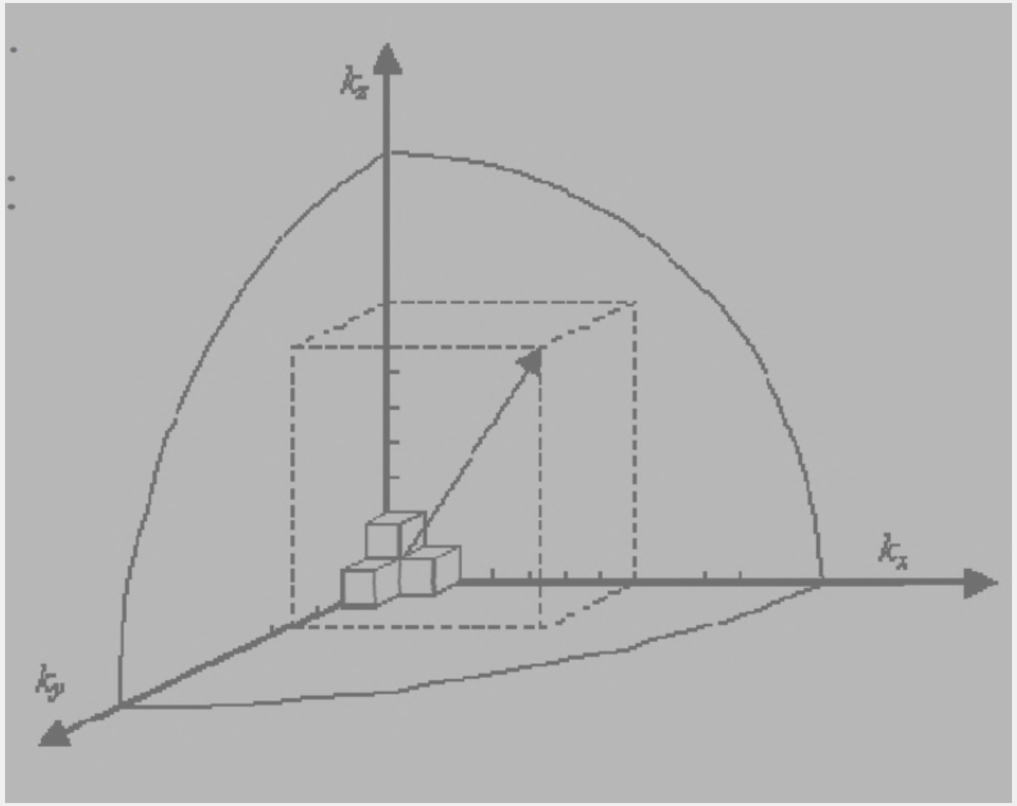
$$k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L} \quad for\ n = \pm 1, 2, 3....$$

# Derivation of density of state of Quantum well (2D)

Recalling from the density of states a 3D crystal derivation.
K-space Volume of single state cube in k-space:

$V_{\text{single state}} = (\pi/a)\,(\pi/b)\,(\pi/c) = (\pi^3/V)$,
here V= volume of the crystal

$V_{\text{single state}}$ is the smallest unit in k-space single-state and is required to hold a single electron



# Derivation of density of state of Quantum well (2D)

Volume of sphere in k-space is:

$$V_{sphere} = \frac{4\pi k^3}{3}$$

Here, $k = \sqrt{\frac{2mE}{\hbar^2}}$

Number of filled state in K-space (N):

$$N = \frac{V_{Sphere}}{V_{single-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2}\right)$$

A factor of two is added to account for the two possible electron spins of each solution.

Correction factor for redundancy in counting identical states +/- $n_x$, +/- $n_y$, +/- $n_z$

# Derivation of density of state of Quantum well (2D)

Number of filled state in K-space (N):

$$N = \frac{\frac{4}{3}\pi k^3}{\frac{\pi^3}{L^3}} \times 2 \times \left(\frac{1}{8}\right) = \frac{4\pi k^3 L^3}{3\pi^2}$$

For calculating the density of states for a 2D structure (i.e. quantum well), we can use a similar approach, the previous equations change to the following:

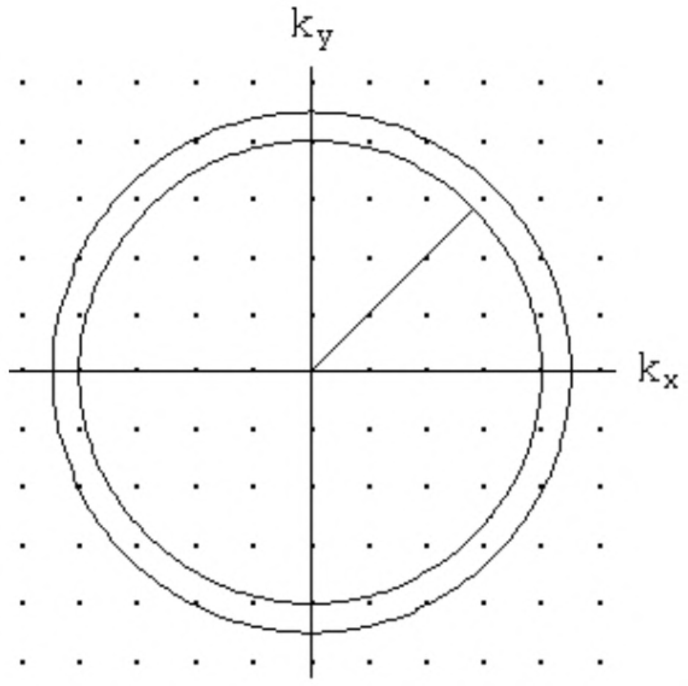
k- space Volume of single state cube in k-space (2D):

$$V_{single-state} = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right) = \left(\frac{\pi^2}{V}\right) = \left(\frac{\pi^2}{L^2}\right)$$

# Derivation of density of state of Quantum well (2D)

**k –space Volume of sphere in k-space is**

$$V_{circle} = \pi k^2$$




Number of filled state in K-space (N):

$$N = \frac{V_{circle}}{V_{\sin gle-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2}\right)$$

$$N = \frac{\pi k^2}{\frac{\pi^2}{L^2}} \times 2 \times \left(\frac{1}{4}\right) = \frac{k^2 L^2}{2\pi}$$

# Derivation of density of state of Quantum well (2D)

Number of filled state in K-space (N):

$$N = \frac{\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 L^2}{2\pi} = \frac{mL^2 E}{\hbar^2 \pi}$$

$$\text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Density per unit energy is given by:

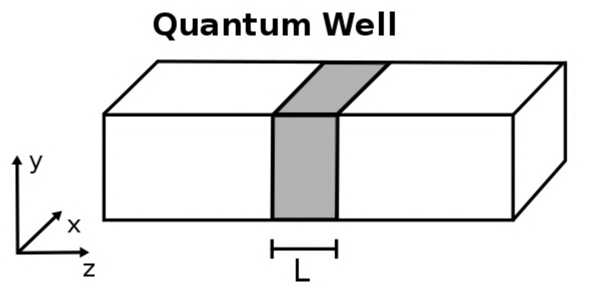
$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{L^2 m}{\pi \hbar^2}$$

# Derivation of density of state of Quantum well (2D)

The density of states per unit area, per unit energy is found by dividing  by $L^2$ (area of the crystal).

$$g(E)_{2D} = \frac{\frac{L^2 m}{\pi\hbar^2}}{L^2} = \frac{m}{\pi\hbar^2}$$

It is significant that the 2D  density of states does not depend on energy. Immediately, as the  top of the energy-gap is reached, there is a significant number of  available states.

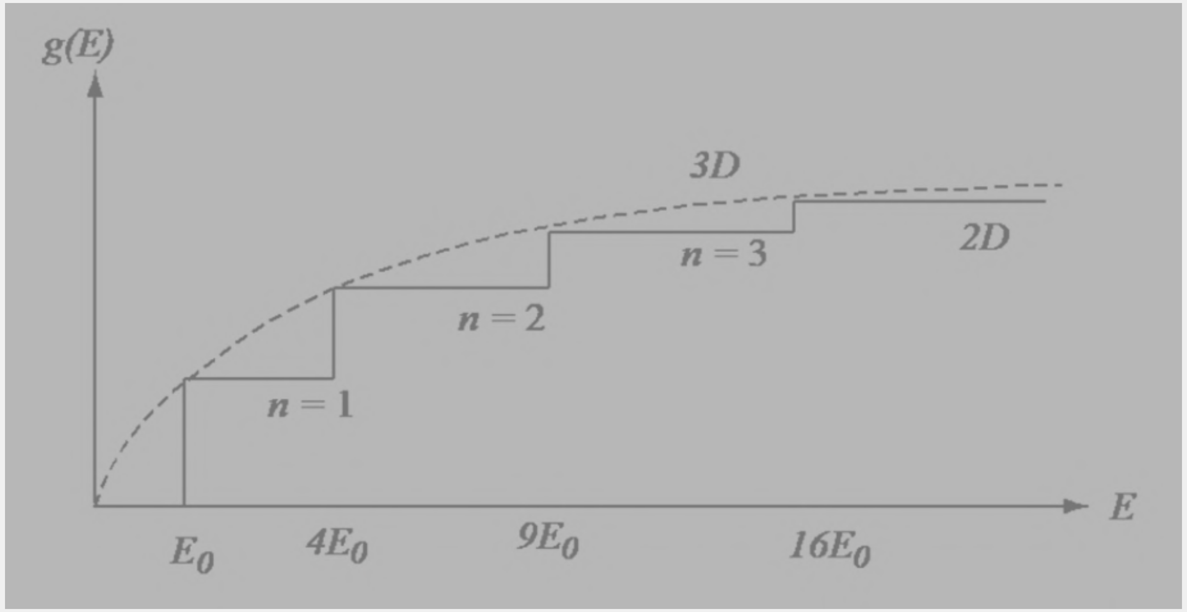



To convert  g(E) which is the density of states per unit area, to a density of states per unit  volume, one must divide by an appropriate length in the *z*-direction, in this case L .

# Derivation of density of state of Quantum well (2D)

Density of states per unit volume, per unit energy is:

$$g(E) = \frac{m}{\Pi \hbar^2 L}$$




Density of states for a quantum well (2D)

The confined energy $E_0$ is defined as $n$th subband energy in the $z$-direction

$$E_{c,n} = \frac{\hbar^2 k_z^2}{2m_z} = \frac{\hbar^2 n^2 \pi^2}{2m_z d^2}$$

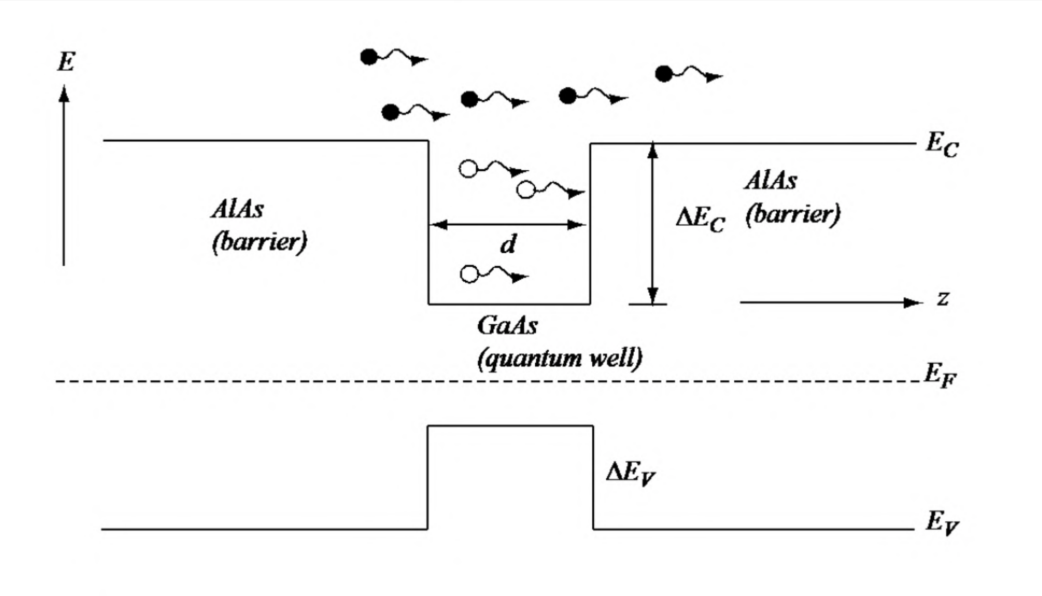
# Applications of Quantum well (2D)

1. Quantum wells are used widely in diode lasers, including red lasers for DVDs and laser pointers, infra-red lasers in fiber optic transmitters, or in blue lasers.
2. They are also used to make HEMTs (high electron mobility transistors), which are used in low-noise electronics.
3. Quantum well infrared photodetectors are also based on quantum wells and are used for infrared imaging.

# Problem

**How to develop a quantum well?**

A quantum well can be formed by sandwiching a thin film between two other materials. For example, a thin layer of GaAs can be sandwiched between two AlAs layers. Both GaAs and AlAs are semiconductors. AlAs has a larger bandgap (2.17 eV) than GaAs (1.42 eV). Quantum confinement of an electron within the thin layer of GaAs will happen if its energy is below that of the conduction band edge in AlAs. This is a compositional quantum well. The barriers prevent the transmission of low energy electrons, and allow only high energy electrons.




Band-edge diagram for a typical GaAs/AlAs quantum well

# Problem

A quantum well of GaAs (gallium arsenide) with the DOS effective mass of 0.07 me is used for a laser, estimate the first three subband energy levels at k = 0 for the quantum width of 60 Å assuming the infinite quantum-well barriers and the electron mass in the z-direction is equal to the DOS effective mass (for a cubic crystal)

**Solution**:

At $k = 0$, the $n$th subband energy with the infinite quantum well barriers is

$$E = \frac{\hbar^2 n^2 \pi^2}{2 m_d^* d^2}$$

For $n = 1$

$$E = \frac{\left(6.626\times10^{-34}\,Js/2\pi\right)^2\left(1^2\right)\pi^2}{2\left(0.07\times9.1093\times10^{-31}\,kg\right)\left(60\times10^{-10}\,m\right)^2\left(1.6021\times10^{-19}\,J/eV\right)} = 0.149eV$$

Likewise,

$E = 0.597\ eV$ for $n = 2$

$E = 1.343\ eV$ for $n = 3$

# References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